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The Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multipathway Chemicals (SHEDS-Multimedia):Dietary Module

SHEDS-Dietary version 1

Quick Start Guide

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1 Purpose of this Quick Start Guide

SHEDS-Dietary is the dietary exposure module of the SHEDS-Multimedia exposure model. It provides a flexible framework for stochastic simulation of population exposures to single or multiple chemicals in food. This Quick Start guide is intended for persons familiar with dietary exposure and risk assessment who would like to quickly learn how to use SHEDS-Dietary via a hands-on approach. This guide presents a quick introduction to the SHEDS model's capabilities and the basic steps required to initialize and run a SHEDS exposure simulation, as demonstrated through an example tutorial case study.

This guide assumes the user is familiar with the general features of the SAS software program. More detailed instructions, scientific explanations, file formats, relevant references, and case studies are available in the SHEDS-Dietary User Guide and Technical Manual. In this Quick Start Guide, readers will be directed to the relevant sections of these additional manuals for more information. This manual assumes that the user has already downloaded and installed the SHEDS-Dietary model (**see Chapter 2** of the SHEDS-Dietary User Guide).

2 Introduction to the SHEDS-Dietary Module

SHEDS-Dietary is a stochastic dietary exposure model that can be used to estimate population estimates of dietary exposure, based on food consumption data from either the United States Department of Agriculture's Continuing Surveys of Food Intake by Individuals (CSFII) for the years 1994-1996 and 1998 or the National Health and Nutrition Examination Survey (NHANES) What We Eat In America (WWEIA) study. Exposure is determined from food consumption through the breakdown of foods to food commodities via recipes, followed by stochastic assignment of chemical residues to food commodities.

SHEDS-Dietary Version 1 is a stand-alone module that can be used in conjunction with the SHEDS-Multimedia Version 4 residential module (also referred to as 'SHEDS'), a sophisticated but user-friendly cumulative human exposure model for chemicals contacted in a residential setting .

Dietary exposure simulations performed using the stand-alone SHEDS-Dietary interface. The interface provides a user-friendly environment for:

- Creating the required SHEDS-Dietary input files, including creation of residue distribution data, assignment of residue distributions to food commodities, and definition of population risk parameters

- Running the SHEDS-Dietary model
- Viewing the model output in chart, graph, and tabular form

The main features of the SHEDS algorithms include:

- Ability to model single (aggregate) or multiple (cumulative) chemical exposures
- Cross-sectional and longitudinal analysis capabilities
- Consideration food, indirect water, and direct water consumption
- Ability to use custom food chemical residue information, or to use information from the Pesticide Data Program (PDP) database

SHEDS results can be used to assess:

- Food and drinking water exposures for individuals
- Ranges and distributions of population dietary exposures
- Key factors and contributions of food types and chemicals to total exposures
- Uncertainties in exposure estimates

3 Steps in Creating and Running a SHEDS-Dietary Simulation

The following are the main steps the user will take in setting up and running a SHEDS dietary exposure simulation (i.e. "model run"). The majority these steps can be accomplished via the SHEDS user interface:

1) **Define the Run**. The user will give the simulation a name and tell SHEDS where to store all input files and results associated with the simulation.

2) **Create Residue Information.** Residue concentrations can reside in text residue data files ("RDF files") associated with food commodities, or created within SHEDS from the PDP database.

3) **Specify the Main Simulation Settings**. For example: Single chemical or multichemical run? Single-day (cross-sectional) or longitudinal simulation? Food consumption only or food and drinking water consumption? What type of residue data will be used (are the data in text RDF files, or have the data been created within SHEDS from the PDP database?)

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4) **Assign Residue Information to Food Commodities.** If the residue concentrations are stored in RDF files, the user will use the interface to assign each RDF file to single or multiple food commodities.

5) **Finalize the Run Settings and Run the Simulation.** The user will be ask to confirm a number of run settings or file locations, enter risk parameters, and run the simulation.

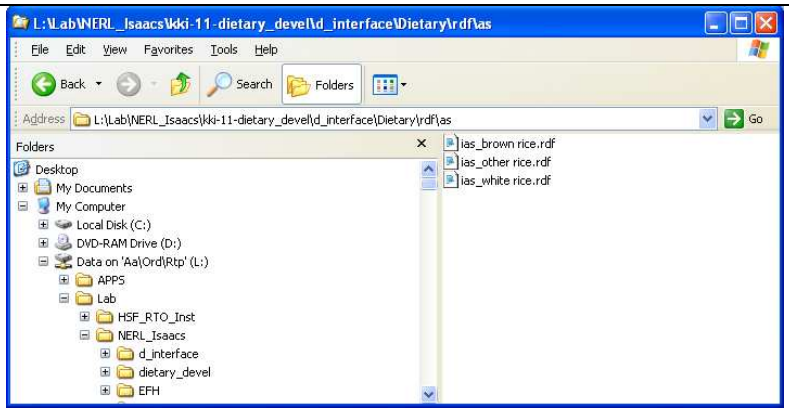
6) **Pre-Process the Model Output Data.** The user will enter settings that will determine output file names, and contribution analyses. Distributions of exposures and summary tables are created.

7) **View the Results.** The user may use the built-in tools provided by SHEDS to view results for the population or for individuals.

The following tutorial is designed to guide the user through these steps for a simple, single-chemical, cross-sectional, SHEDS-Dietary run, in which the residue concentration data are stored in RDF files. Other case study tutorials for multichemical and longitudinal runs are provided in **Chapter 7** of the SHEDS-Dietary User Guide.

4 Example Tutorial Case Study: Arsenic Exposure from Rice Consumption

This case study demonstrates the steps in creating a single chemical, cross-sectional run for arsenic. The example chemical is arsenic (As) and it is assumed that all exposure is due to consumption of different forms of rice. The steps in setting up the run are enumerated below, accompanied by a corresponding screenshot.

Instructions	Associated Screenshot
1) Create the residue (RDF) files of interest for the chemical. In this tutorial, residue files were created for different rice food commodities using a plain-text editor. Store all the residue files in a single directory, under the SHEDS main directory tree. These example files are included in the SHEDS-Dietary package in the directory ".\ **D_interface\Dietary\rdf\as",** where .\ designates the root SHEDS installation directory.	

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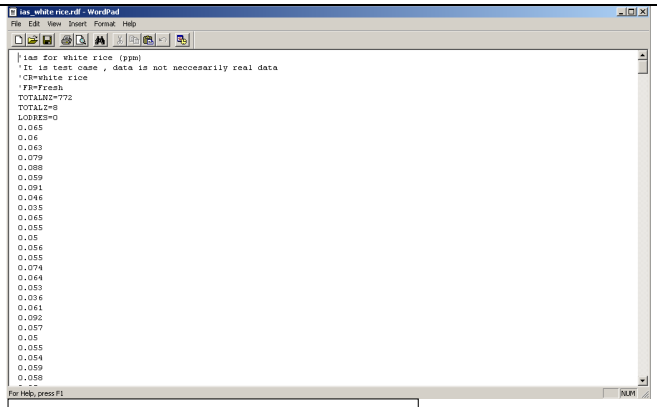
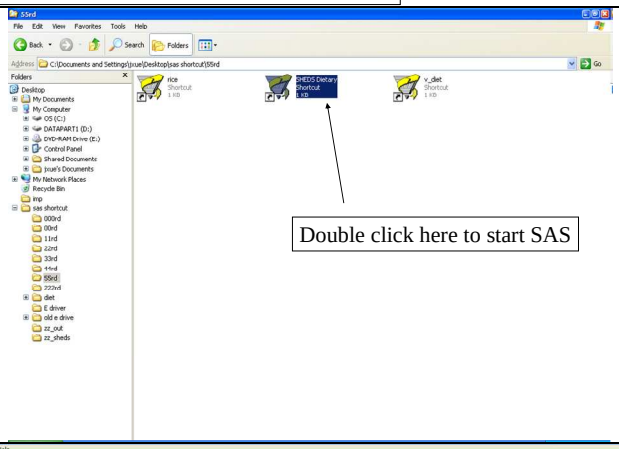
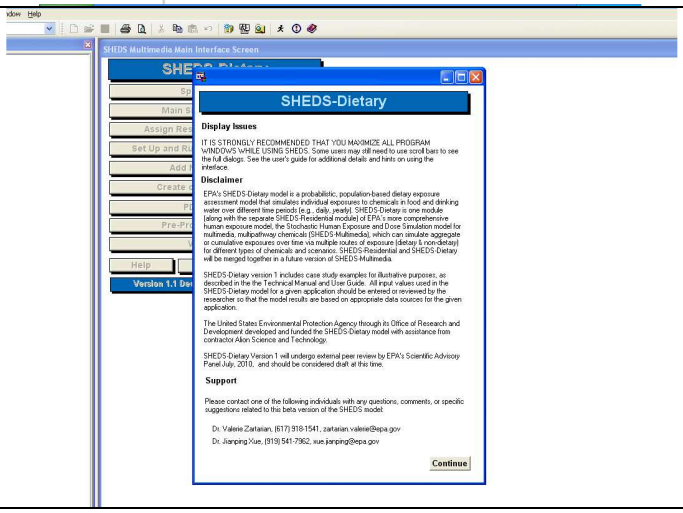
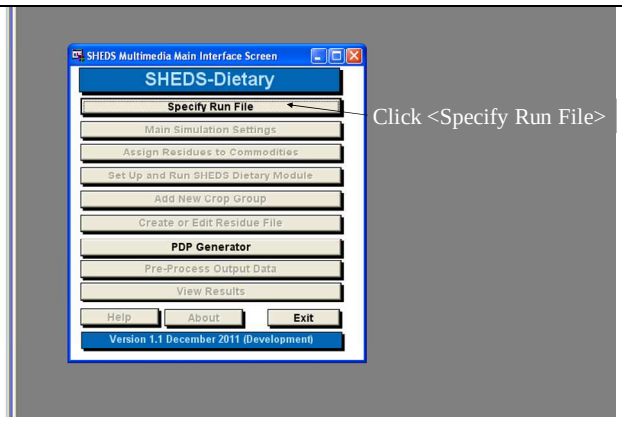
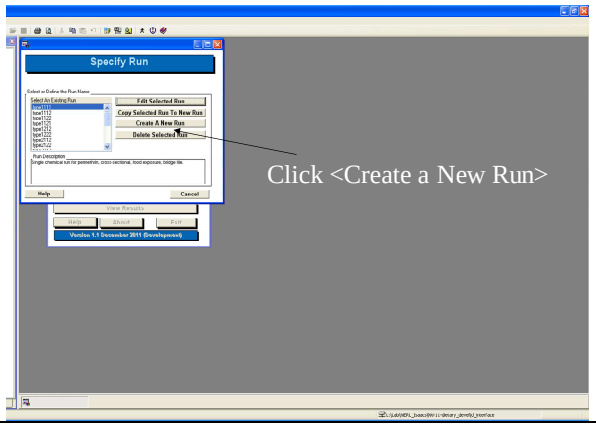
2) An example residue file is shown for white rice. The files follow the format described in detail in **Section 5.5.2 of the SHEDS-Dietary User Guide**. The files can also be created with the SHEDS **Create or Edit Residue Data** utility, described in detail in **Section 5.5 of the SHEDS-Dietary User Guide**	 Example RDF file for white rice for As
3) Initiate a SHEDS-Dietary session by double-clicking the SHEDS-Dietary SAS shortcut icon.	 Double click here to start SAS
4) The SHEDS disclaimer screen appears first; select <Continue> to proceed to the main SHEDS screen.	

5) Select <Specify Run File>, <Create New Run File> to initiate the creation of a new run for arsenic. Detailed instructions for specifying a run are provided in **Section 5.3 of the SHEDS-Dietary User Guide**	 

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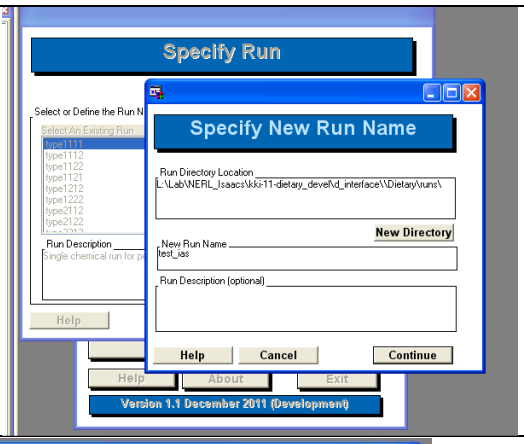
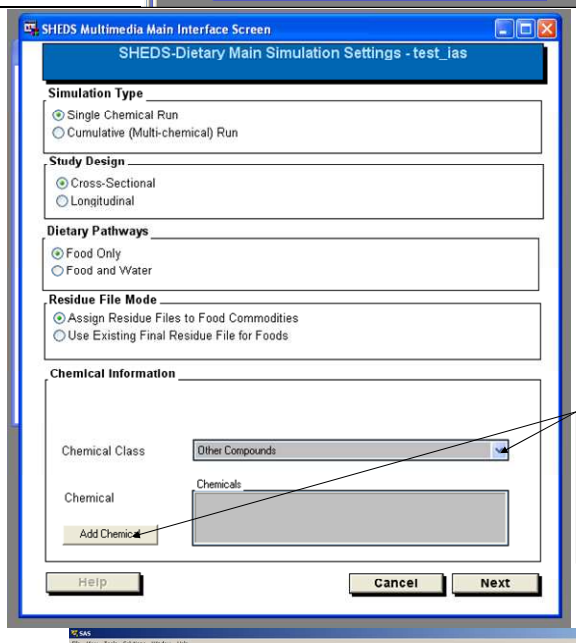
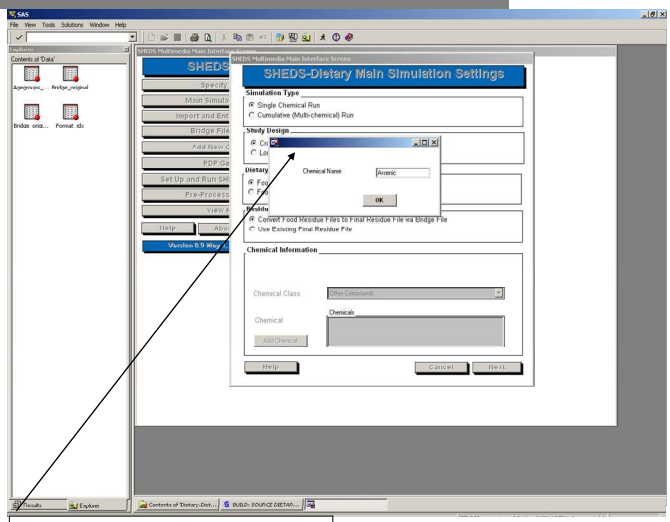
6) Enter the name of the new run as "test_ias" when prompted. Click <Continue>. This will create a new directory in the SHEDS Run Directory (which by default will be ".\d_interface\Dietary\Runs," although the user may change it) for storing the run inputs and outputs.	
7) The Main Simulation Settings button will now be enabled. Select it and the Main Simulation Settings screen will appear. Use the defaults for Simulation Type, Study Design, Dietary Pathways, and Residue File Mode. Select "Other Compounds" for the Chemical Class in the Chemical Information box. Click the "Add Chemical" button. Enter "arsenic". Click OK. Keep all other default settings and select <Next>. This will define a single chemical, cross-sectional simulation of food exposure. In this run, food residue files will be assigned to food commodities. Detailed instructions for specifying main simulation settings are provided in **Section 5.4 of the SHEDS-Dietary User Guide**	 Select "Other Compounds" then click <Add Chemical>  Enter "Arsenic" then click <OK>
8) The second Main Simulation Settings screen appears upon completion of the previous step.	

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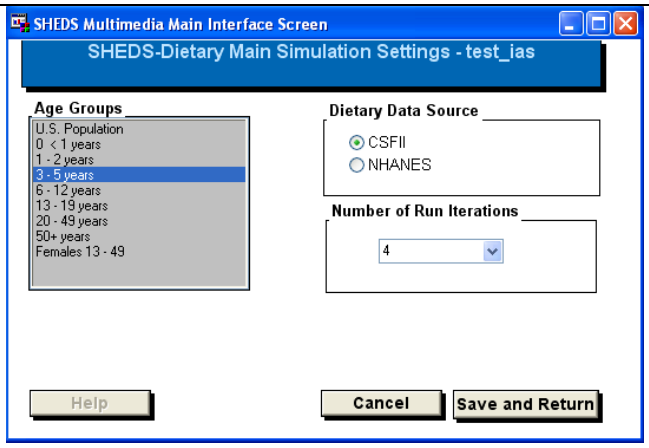
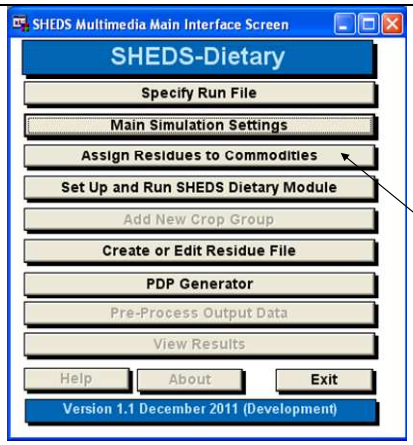
select "4" as the number of run interations and click <Save and Return>. The options on this screen are discussed in **Section 5.4 of the SHEDS-Dietary User Guide.**

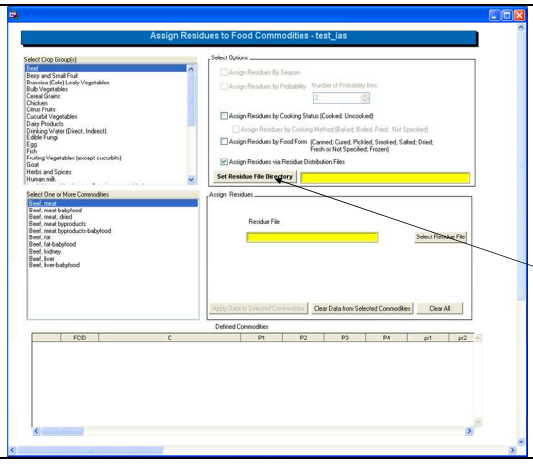


9) When SHEDS returns to the Main Screen, click the Assign Residues to Commodities button. This button will open the screen the user will use to assign RDF (residue) files to individual food commodities. These may be assigned by food form or cooking method if the user desires, but typically residues are assigned to all forms of a commodity. The options and features of this Screen are described in **Section 5.6 of the SHEDS-Dietary User Guide.**



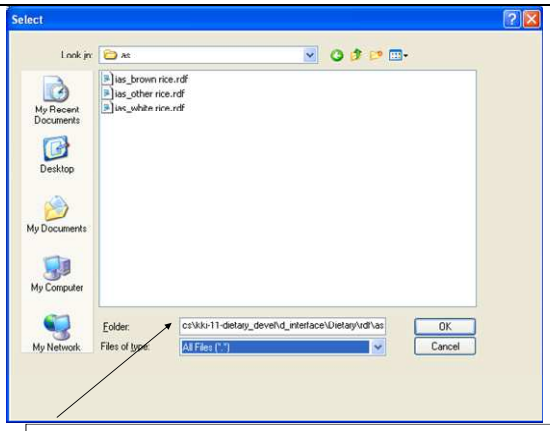
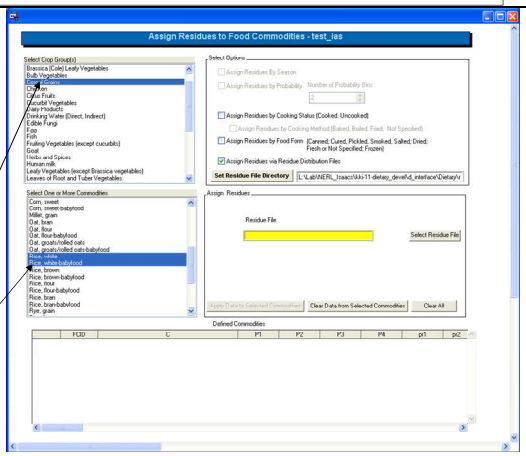
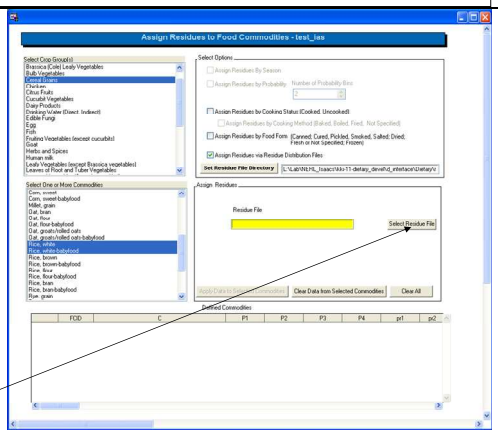
Select <Assign Residues to Commodities>

10) Select the directory where the arsenic residue files are located by clicking the <Set Residue File Directory> button. The files are located in <install>/Dietary/rdf/as, as defined in Step 1 (the folder name will be different than the one shown in the figure below, since different user's installation folder names may differ).



Select <Set Residue File Directory>

US EPA ARCHIVE DOCUMENT

	 Select the directory ".\d_interface\dietary\rfd\as" where "." indicates the SHEDS installation directory
11) Select the Crop Group "Cereal Grains." This will populate the food commodity list. Select the food commodities "Rice, white" and "Rice, white, babyfood." Hold the control button down while clicking to select multiple commodities.	 Select "Cereal Grains" and then select the white rice commodities.
12) Now click <Select Residue File>, will open window with a list of the available RDF files in the specified directory. Select the RDF file "ias_white rice.rdf" and click <OK>.	 Click <Select Residue File>

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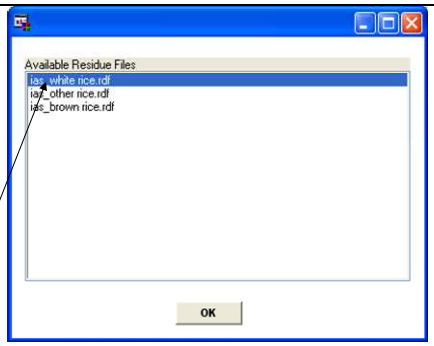
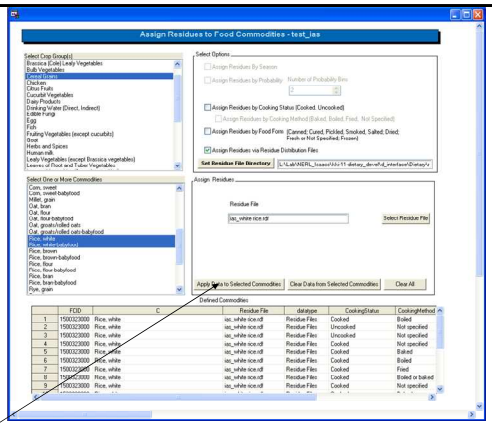
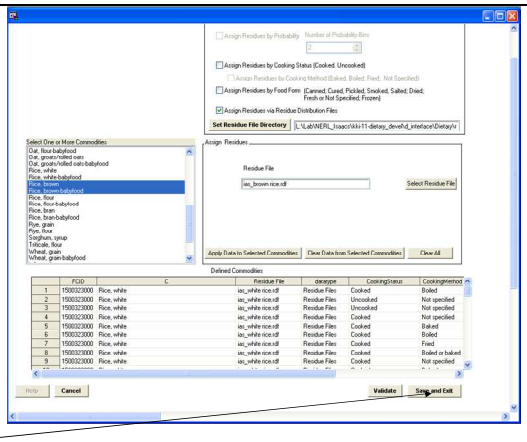
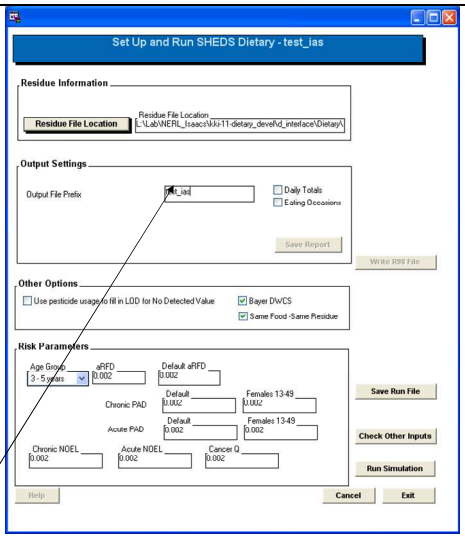
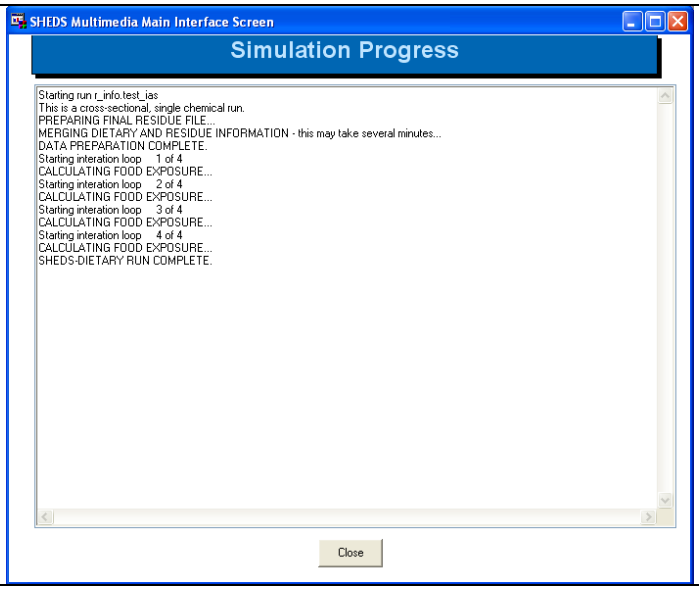
	 Select the residue file “ias_white rice.rdf”
13) Click <Apply Data to Selected Commodities> to assign the selected residue file to the selected food commodities. This will populate a list in the Defined Commodities window describing the linkages. This is for the convenience of the user. Notice that in this example the RDF files are assigned to all Food Forms and Cooking Methods.	 Click <Apply Data to Selected Commodities>
14) Populate the other rice commodities with the appropriate Residue files by repeating Steps 11-13 for additional commodities. Assign the file "ias_brown rice.RDF" to the brown rice commodities, and then assign "ias_other rice.RDF" to all remaining rice commodities.	
15) Click <Save and Exit> once all the rice commodities are assigned residues.	 Click <Save and Exit>

16) Select the <Set Up and Run SHEDS-Dietary> button from the Main SHEDS screen. Provide a prefix for the run ("test_ias_"). This will be used to label output data, which will be stored in the Run directory for the run. Enter the desired risk (toxicological) parameters (or use the ones provided in the example), and then click <Save Run File> to save the Run File. The simulation is then run by selecting <Run Simulation>. Details on this screen and its options are provided in **Section 5.7 of the SHEDS-Dietary User Guide.**	 Enter Prefix for run ("test_ias"). Click <Save Run File> then <Run Simulation>
17) Monitor the progress of the SHEDS run via the Run Progress dialog. When the run is done, select <Close>.	

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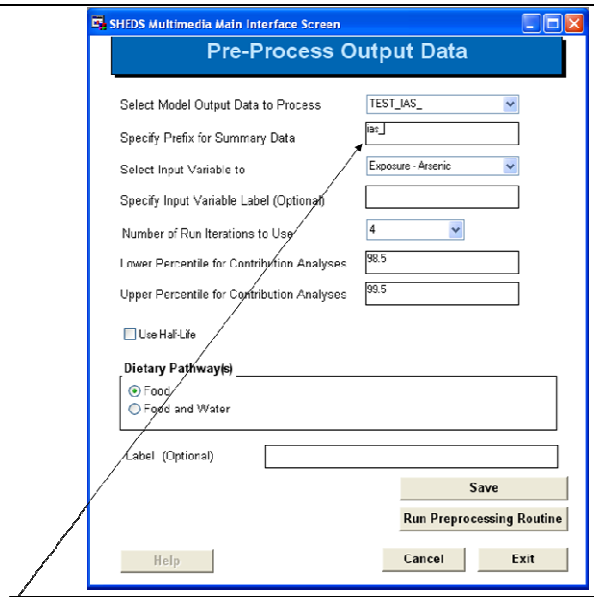
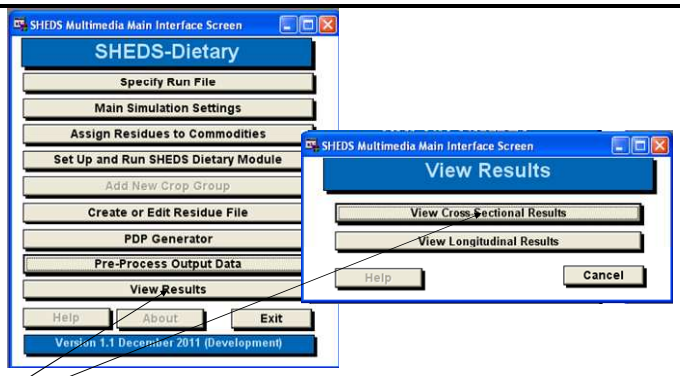
18) The Pre-Process Output Data screen will open automatically. Select the prefix of the run to be preprocessed (test_ias_) and a prefix for the summary data (also test_ias_). (Everything except the prefix should be the default). Also select the number of iteration runs to use, and the upper and lower percentiles to be used for the contribution analyses. Then, click the Run Preprocessing Routine button, and then the OK button. Details on this screen and its options are provided in **Section 5.8 of the SHEDS-Dietary User Guide.**



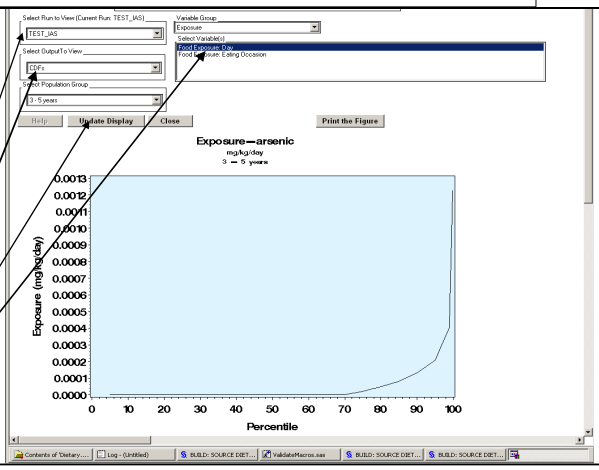
Enter prefix for summary data ("ias_"). Click <Save> then <Run Preprocessing Routine>. When done, <Exit>.

19) Click on the <View Results> button to display the View Results selection screen. Select <View Cross-Sectional Data>. Details on this screen and its options are provided in **Section 5.9 of the SHEDS-Dietary User Guide.**



Click <View Results>, and then <View Cross-Sectional Results>.

20) The main View Cross-Sectional Results screen will now appear. Select the run of interest (TEST_IAS) from the run selection list (the name will appear without the trailing underscore). Select "CDFs" as the output to view, and highlight the variable Food Exposure:Day. Selecting <Update Display> will update the figure with the selected options. In this way, different output tables and graphs can be generated.



Select the run "test_ias", "CDFs" as output to view, "Food Exposure: Day" as variable, and click <Update Display>

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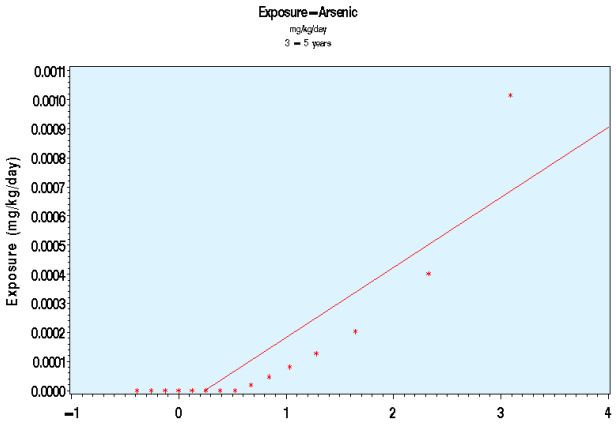
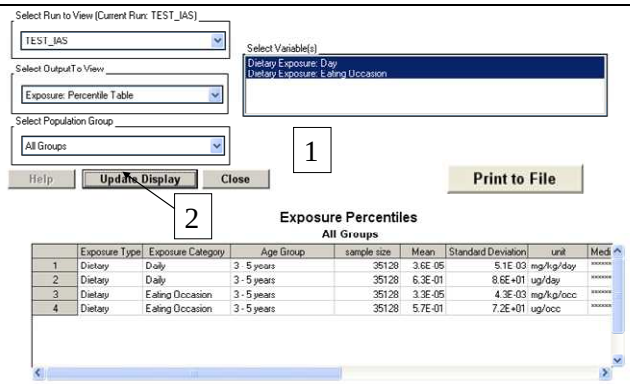
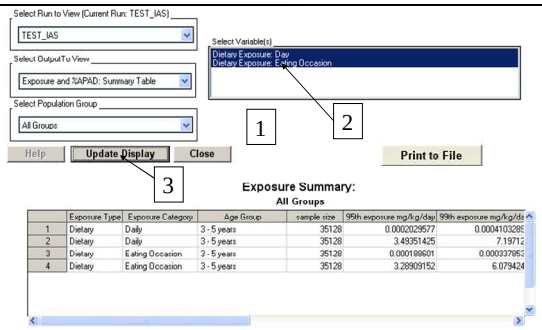
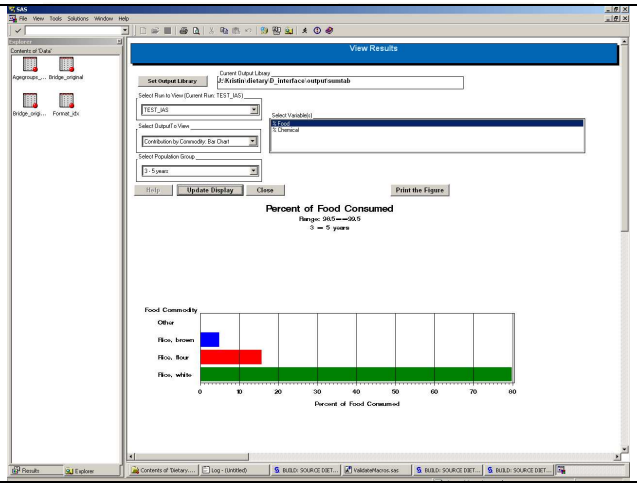
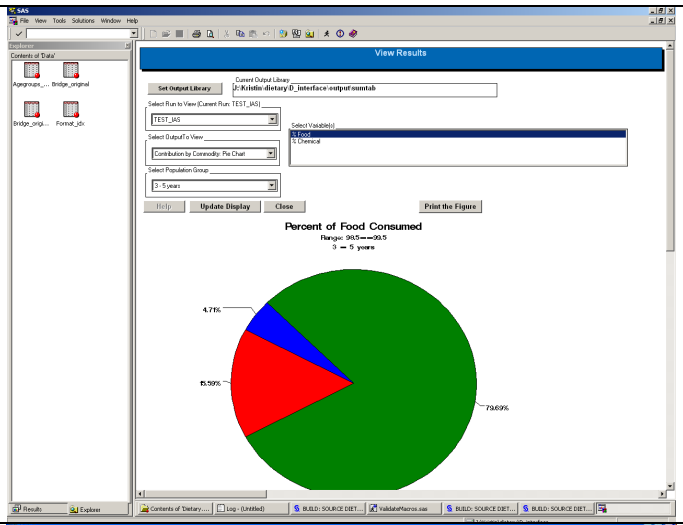
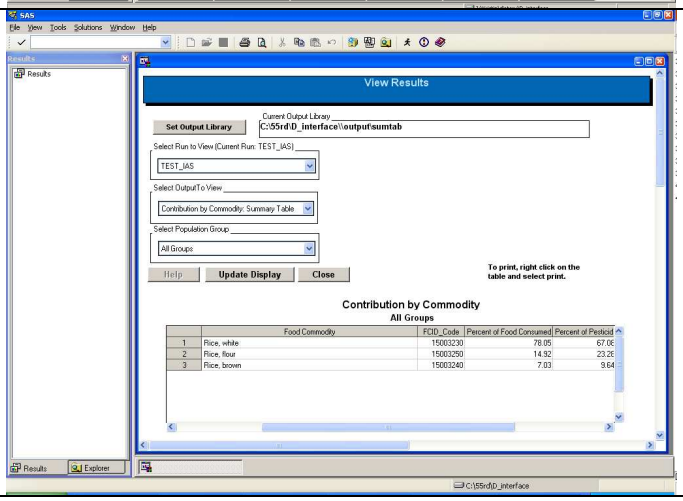
21) Select "Z-score plot" as the output to view and click <Update Display>. This will generate the z-score plot for arsenic exposure.	
22) Select "Exposure Percentile Table" as the output to view, highlight both available variables, and click <Update Display>. This will generate the requested table for the selected variables.	
23) Repeat this process by selecting "Exposure and %APAD: Summary Table," selecting the two available variables, and again updating the display.	
24) Selecting "Contribution by Commodity: Bar Chart" as output to view and % Food as the variable produces a bar chart of % food consumed by commodity. A plot of the contribution of food types to total chemical exposure can also be generated by selecting % Chemical as the variable.	

25) Analogous Pie charts can also be displayed by selecting "Contribution by Commodity: Pie Chart."	
26) Finally, a contribution table can be created by selecting "Contribution by Commodity: Summary Table" as the output to view.	

5 Recommended Next Steps

Once the new user has worked through this tutorial, it is recommended that they read through the User's Guide to better understand the capabilities and options of SHEDS. Additional Case Studies, including case studies for multichemical and longitudinal studies, and how to generate final SHEDS residue files from the PDP database, are provided in **Section 7 of the SHEDS-Dietary User Guide.**

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